Motion of electrons in adiabatically perturbed periodic structures

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Summary. We study the motion of electrons in a periodic background potential (usually resulting from a crystalline solid). For small velocities one would use either the non-magnetic or the magnetic Bloch hamiltonian, while in the relativistic regime one would use the Dirac equation with a periodic potential. The dynamics, with the background potential included, is perturbed either through slowly varying external electromagnetic potentials or through a slow deformation of the crystal. In either case we discuss how the Hilbert space of states decouples into almost invariant subspaces and explain the effective dynamics within such a subspace.

1 Introduction

In a crystalline solid the conduction electrons move in the potential created by the ions and the core electrons. Somewhat mysteriously and linked to the Pauli exclusion principle, the Coulomb repulsion between conduction electrons may be ignored, within a good approximation. Thereby one arrives at a fundamental model of solid state physics, namely an ideal Fermi gas of electrons subject to a periodic crystal potential. Let Γ be the periodicity lattice. It is a Bravais lattice and generated through the basis $\{\gamma_1, \gamma_2, \gamma_3\}$, $\gamma_j \in \mathbb{R}^3$, as

$$\Gamma = \{\gamma = \sum_{j=1}^{3} \alpha_j \gamma_j \quad \text{with } \alpha \in \mathbb{Z}^3\}\,. \tag{1.1}$$

The crystal potential V_Γ is then Γ-periodic, i.e., $V_\Gamma : \mathbb{R}^3 \to \mathbb{R}$ and $V_\Gamma(x+\gamma) = V_\Gamma(x)$ for all $\gamma \in \Gamma$, and the electrons are governed by the one-particle hamiltonian

$$H_{\mathrm{SB}} = -\frac{1}{2}\Delta_x + V_\Gamma\,. \tag{1.2}$$

H_{SB} is the (Schrödinger)–Bloch hamiltonian. A wave function $\psi_t \in L^2(\mathbb{R}^3)$ evolves in time according to the Schrödinger equation

$$i\frac{\partial}{\partial t}\psi_t = H_{\mathrm{SB}}\psi_t\,. \tag{1.3}$$

We have chosen units such that the mass of an electron $m_{\mathrm{e}} = 1$ and $\hbar = 1$. The electron charge, e, is absorbed in V_Γ. Since V_Γ is periodic, electrons move ballistically with an effective dispersion relation given by the Bloch energy bands E_n, see below for a precise definition. E_n is periodic with respect to the lattice Γ^* dual to Γ, $E_n(k+\gamma^*) = E_n(k)$ for all $\gamma^* \in \Gamma^*$, $k \in \mathbb{R}^3$. This feature makes the dynamical properties of a Bloch electron very different from a massive particle with dispersion $E_{\mathrm{free}}(k) = \frac{1}{2}k^2$ valid in case $V_\Gamma = 0$.

The thermodynamics of the electron gas is studied taking H_{SB} as a starting point. Dynamically, however, one wants to probe the response of the electrons to external forces which very crudely come in two varieties.

(i) *External electromagnetic potentials.* Electrostatic potentials manufactured in a lab have a slow variation on the scale of the lattice Γ. Therefore we set $V_{\mathrm{ext}}(x) = e\phi(\varepsilon x)$, e the charge of the electron, with ε a dimensionless parameter and ϕ independent of ε. $\varepsilon \ll 1$ means that the potential V_{ext} has a slow variation when measured with respect to the lattice spacing of Γ. Note that the electrostatic force is $\mathcal{O}(\varepsilon)$ and thus weak. External magnetic fields on the other hand can be so strong that the radius of gyration is comparable to the lattice spacing. It then makes sense to split the vector potential as $A_0 + A_{\mathrm{ext}}$, where $A_0(x) = -\frac{1}{2}B_0 \wedge x$ with $B_0 \in \mathbb{R}^3$ a constant magnetic field. Included in H_{SB}, this yields the magnetic Bloch hamiltonian

$$H_{\mathrm{MB}} = \frac{1}{2}(-i\nabla_x - A_0)^2 + V_\Gamma\,. \tag{1.4}$$

A_{ext} is a probing vector potential in addition to A_0. A_{ext} is slowly varying on the scale of the lattice, $A_{\mathrm{ext}}(x) = A(\varepsilon x)$ with A independent of ε, and the corresponding magnetic field is small of order ε. Including all electromagnetic potentials, for simplicity with the electric charge absorbed into A and ϕ, the hamiltonian becomes

$$H = \frac{1}{2}\big(-i\nabla_x - A_0(x) - A(\varepsilon x)\big)^2 + V_\Gamma(x) + \phi(\varepsilon x)\,. \tag{1.5}$$

(ii) *Mechanical forces.* The crystal lattice can be deformed through external pressure and shear. Thereby an electric polarization is induced, an effect which is known as piezoelectricity. If charges are allowed to flow, in this way mechanical pressure can be transformed into electric currents. The mechanical forces are time-dependent but slow on the typical time-scale of the electrons. Therefore in (1.2) $V_\Gamma(x)$ is replaced by $V_{\Gamma(\varepsilon t)}(x, \varepsilon t)$. $\Gamma(\varepsilon t)$ is the instantaneous periodicity lattice and is defined as in (1.1). $V_{\Gamma(t)}$ is space-periodic, i.e. $V_{\Gamma(t)}(x+\gamma, t) = V(x,t)$ for all $\gamma \in \Gamma(t)$. The special case of a time-independent lattice, $\Gamma(t) = \Gamma$, but a still slowly in time varying crystal potential is also of interest. For example, one may imagine a unit cell with

two nuclei. If the two nuclei are displaced relative to each other, then Γ remains fixed while the crystal potential in the unit cell changes with time. The resulting piezoelectric hamiltonian reads

$$H_{\mathrm{PE}}(t) = -\frac{1}{2}\Delta_x + V_{\Gamma(\varepsilon t)}(x, \varepsilon t)\,. \tag{1.6}$$

Our general goal is to understand, in each case, the structure of the solution of the time-dependent Schrödinger equation for small ε. Obviously, H in (1.5) is a space-adiabatic problem, while (1.6) corresponds to a time-adiabatic problem. However in the latter case it turns out to be profitable to transform to a time-independent lattice, say $\Gamma(0)$. Then also terms varying slowly in space are generated. Thus, in the general case the full power of the space-adiabatic perturbation theory [PST03a, Teu03] will be needed. A word of caution must be issued here for the magnetic Bloch hamiltonian. To use the methods from [PST03a] in this context, the unperturbed Hamiltonian must be periodic, which is the case only if the magnetic flux per unit cell is rational. One can then define an enlarged magnetic unit cell such that H_{MB} is invariant with respect to magnetic translations. If the magnetic flux is not rational, the crutch is to include in A_0 a nearby rational flux part of the magnetic field, with a small denominator, and to treat the remainder as A_{ext}.

To achieve our goal, depending on the context we use one of the periodic hamiltonians as backbone. The periodic hamiltonian is denoted by H_{per} with H_{per} either H_{SB}, or H_{MB}, or H_{PE} at fixed t, or H_{LS} from (1.8), or H_{DB} from (1.9). As explained below, the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)$ then splits as $\mathcal{H} = \bigoplus_{n=0}^{\infty} \mathcal{H}_n$, where n is the band index. Each subspace $\mathcal{H}_n$ is invariant under $\exp[-itH_{\mathrm{per}}]$ and H_{per} restricted to $\mathcal{H}_n$ is unitarily equivalent to multiplication by $E_n(k)$. $E_n(k)$ is the effective hamiltonian associated to the n-th band. The complexity of the full problem has been reduced substantially, since only a single band dynamics has still to be studied. Modifying H_{per} such that it becomes slowly varying in space-time is, vaguely speaking, a small perturbation. Thus one would expect that the invariant subspace $\mathcal{H}_n$ is to be substituted by a slightly tilted subspace. On this subspace $E_n(k)$ will turn into a more complicated effective hamiltonian. The difficulty is that, while the dynamics generated by H_{per} can be computed by solving a purely spectral problem, none of the perturbed hamiltonians can be understood in this way. In particular, one has to spell out carefully over which time scale the slightly tilted subspace associated to $\mathcal{H}_n$ remains approximately invariant and in what sense the dynamics generated by the effective hamiltonian approximates the true time evolution.

To lowest order the effective hamiltonian can be guessed from elementary considerations and belongs to a standard tool of solid state physics [AM76]. The guess provides however little hint on the validity of the approximation. There one needs a mathematical theorem which states precise conditions on

the initial wave function and provides an error bound, from which the time scale for validity can be read off.

Under the header "geometric phase" physicists and quantum chemists have realized over the past twenty years, say, that the first order correction to the effective hamiltonian carries a lot of interesting physics, see [BMKNZ03] for a recent comprehensive overview. For the magnetic Bloch hamiltonian the first order correction yields a Hall current proportional to the Chern number of the magnetic Bloch vector bundle. Similarly, the modern theory of piezoelectricity, expresses the piezocurrent as an integral of the Berry connection over the Brillouin zone, see King-Smith, Vanderbilt [KSV93] and Resta [Res94]. First order effective Hamiltonians are no longer guessed so easily and it is convenient to have the systematic scheme [PST03a] available.

In nature electrons are spin $\frac{1}{2}$ particles. The wave function is thus $\mathbb{C}^2$-valued and the hamiltonian in (1.5) is modified to

$$H = \frac{1}{2}\big(-i\nabla_x - A_0(x) - A(\varepsilon x)\big)^2 + V_\Gamma(x) + \phi(\varepsilon x) - \frac{1}{2}\sigma\cdot\big(B_0 + \varepsilon B(\varepsilon x)\big) \quad (1.7)$$

with $B = \nabla \wedge A$ for the slowly varying part of the magnetic field. Here $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ is the 3-vector of Pauli spin matrices. Besides the term proportional to the uniform magnetic field B_0, H acquires a subleading term of order ε. More accurately one may want to include the spin-orbit coupling. The periodic piece of the hamiltonian reads then

$$H_{\mathrm{LS}} = -\frac{1}{2}\Delta_x + V_\Gamma(x) + \frac{1}{4}\sigma\cdot\big(\nabla V_\Gamma(x) \wedge (-i\nabla_x)\big) \quad (1.8)$$

and the slowly varying potential is added as in (1.7) with the additional subleading term $\varepsilon\frac{1}{4}\sigma\cdot(\nabla\phi(\varepsilon x)\wedge(-i\nabla_x))$.

Depending on the crystalline solid, the conduction electrons can move so fast that relativistic corrections become important. On the one-particle level an obvious choice is then the Dirac equation with a periodic potential V_Γ. Wave functions are $\mathbb{C}^4$-valued and the hamiltonian reads

$$H_{\mathrm{DB}} = \beta m_{\mathrm{e}}c^2 + c\alpha\cdot p + V_\Gamma\,, \quad p = -i\nabla_x\,. \quad (1.9)$$

We introduced here the mass, m_{e}, of the electron and the speed of light, c. The 4×4 matrices $\beta, \alpha_1, \alpha_2, \alpha_3$ are standard and defined in [Tha94, Ynd96], for example. Note that the Lorentz frame is fixed by the solid, i.e. by V_Γ.

In fact, the non-relativistic limit for H_{DB} yields the spin-orbit hamiltonian H_{LS} [Tha94, Ynd96]. If $\|V_\Gamma\|$ is bounded, for sufficiently large c, the Dirac hamiltonian H_{DB} has a spectral gap, which widens as $c\to\infty$. Projecting onto the electron subspace, to leading order in $1/c$ one obtains the Pauli-Bloch hamiltonian $-(1/2m_{\mathrm{e}})\Delta_x + V_\Gamma$ with the spin-orbit coupling in (1.8) as a correction of strength $1/(m_{\mathrm{e}}c)^2$. In addition the crystal potential is corrected by $-\Delta_x V_\Gamma(x)/8(m_{\mathrm{e}}c)^2$.

In our contribution we will provide some background on how to establish, including error bounds, the validity of the approximate dynamics as generated

by an effective hamiltonian, including order ε corrections, for most of the models mentioned in the introduction. For this purpose it is necessary to briefly recall the spectral theory for the periodic hamiltonian, which is done in the following section. In the subsequent sections we deal with particular cases in more detail. We start with the non-magnetic Bloch hamiltonian, see (1.5) with $B_0 = 0$. For the magnetic Bloch hamiltonian we explain how $B_0 \to 0$ and $B_0 \to \infty$ may be viewed as particular adiabatic limits. Piezoelectricity is discussed in the last section.

Remark. Our contribution is one part of the research project jointly with S. Bauer and M. Kunze within the Schwerpunkt. Their part will be covered in [BK06]. Both contributions appear now as almost disjoint, which only reflects that we wanted to present a coherent story. The unifying aspect is an adiabatic limit for wave-type evolution equations. In this contribution we stay on the level of effective hamiltonians while in [BK06] one pushes the scheme to the first dissipative correction.

2 The periodic hamiltonians

We consider a general dimension, d, and assume that the periodicity lattice Γ is represented as

$$\Gamma = \left\{ x \in \mathbb{R}^d : x = \textstyle\sum_{j=1}^d \alpha_j \, \gamma_j \ \text{ for some } \alpha \in \mathbb{Z}^d \right\}, \tag{2.1}$$

where $\{\gamma_1, \ldots, \gamma_d\}$ are vectors spanning $\mathbb{R}^d$. We denote by Γ^* the dual lattice of Γ with respect to the standard inner product in $\mathbb{R}^d$, i.e. the lattice generated by the dual basis $\{\gamma_1^*, \ldots, \gamma_d^*\}$ determined through the conditions $\gamma_i^* \cdot \gamma_j = 2\pi\delta_{ij}$, $i, j \in \{1, \ldots, d\}$. The centered fundamental domain M of Γ is defined by

$$M = \left\{ x \in \mathbb{R}^d : x = \textstyle\sum_{j=1}^d \beta_j \, \gamma_j \ \text{ for } \beta_j \in [-\frac{1}{2}, \frac{1}{2}] \right\}, \tag{2.2}$$

and analogously the centered fundamental domain M^* of Γ^*. The set M^* is the *first Brillouin zone* in the physics parlance.

Assumption 1. *The crystal potential $V_\Gamma : \mathbb{R}^d \to \mathbb{R}$ satisfies $V_\Gamma(x + \gamma) = V_\Gamma(x)$ for all $\gamma \in \Gamma$, $x \in \mathbb{R}^d$. V_Γ is infinitesimally bounded with respect to $-\Delta$.*

It follows from Assumption 1 that the periodic hamiltonians discussed below are self-adjoint on the domain of $-\Delta$.

2.1 The Bloch hamiltonian

We consider

$$H = -\frac{1}{2}\Delta + V_\Gamma \, . \tag{2.3}$$

The periodicity of H is exploited through the Bloch-Floquet-Zak transform, or just the Zak transform for sake of brevity [Zak68]. The advantage of such a variant is that the fiber at k of the transformed Hamiltonian operator has a domain which does not depend on k.

The Zak transform is defined as

$$(\mathcal{U}_{\mathrm{Z}}\psi)(k,x) := \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}k\cdot(x+\gamma)}\psi(x+\gamma)\,, \qquad (k,x)\in\mathbb{R}^{2d}, \tag{2.4}$$

initially for a fast-decreasing function $\psi\in\mathcal{S}(\mathbb{R}^d)$. One directly reads off from (2.4) the following periodicity properties

$$\big(\mathcal{U}_{\mathrm{Z}}\psi\big)(k,y+\gamma) = \big(\mathcal{U}_{\mathrm{Z}}\psi\big)(k,y) \quad \text{ for all } \quad \gamma\in\Gamma\,, \tag{2.5}$$

$$\big(\mathcal{U}_{\mathrm{Z}}\psi\big)(k+\lambda,y) = \mathrm{e}^{-\mathrm{i}y\cdot\lambda}\,\big(\mathcal{U}_{\mathrm{Z}}\psi\big)(k,y) \quad \text{ for all } \quad \lambda\in\Gamma^*\,. \tag{2.6}$$

From (2.5) it follows that, for any fixed $k\in\mathbb{R}^d$, $\big(\mathcal{U}_{\mathrm{Z}}\psi\big)(k,\cdot)$ is a Γ-periodic function and can thus be regarded as an element of $\mathcal{H}_{\mathrm{f}} = L^2(M)$. $M = \mathbb{R}^d/\Gamma$ and it has the topology of the d-dimensional torus $\mathbb{T}^d$. On the other side, Equation (2.6) involves a unitary representation of the group of lattice translations on Γ^* (isomorphic to Γ^* and denoted as Λ), given by

$$\tau : \Lambda\to\mathcal{U}(\mathcal{H}_{\mathrm{f}})\,, \quad \lambda\mapsto\tau(\lambda)\,, \quad \big(\tau(\lambda)\varphi\big)(y) = \mathrm{e}^{\mathrm{i}y\cdot\lambda}\varphi(y). \tag{2.7}$$

It is then convenient to introduce the Hilbert space

$$\begin{aligned}\mathcal{H}_\tau &= \big\{\psi\in L^2_{\mathrm{loc}}(\mathbb{R}^d,\mathcal{H}_{\mathrm{f}}):\ \psi(k-\lambda)=\tau(\lambda)\,\psi(k) \qquad \text{for all } \lambda\in\Lambda\big\}\\ &= L^2_\tau(\mathbb{R}^d\,,\ \mathcal{H}_{\mathrm{f}})\,,\end{aligned} \tag{2.8}$$

equipped with the inner product

$$\langle\psi,\,\varphi\rangle_{\mathcal{H}_\tau} = \int_{M^*} dk\,\langle\psi(k),\,\varphi(k)\rangle_{\mathcal{H}_{\mathrm{f}}}\,. \tag{2.9}$$

Obviously, there is a natural isomorphism between $\mathcal{H}_\tau$ and $L^2(M^*,\mathcal{H}_{\mathrm{f}})$ given by restriction from $\mathbb{R}^d$ to M^*, and with inverse given by τ-equivariant continuation, as suggested by (2.6). Equipped with these definitions, one checks that the map in (2.4) extends to a unitary operator

$$\mathcal{U}_{\mathrm{Z}} : L^2(\mathbb{R}^d)\to\mathcal{H}_\tau\cong L^2(M^*,L^2(M)), \tag{2.10}$$

with inverse given by

$$(\mathcal{U}_{\mathrm{Z}}^{-1}\varphi)(x) = \int_{M^*} dk\,\mathrm{e}^{\mathrm{i}k\cdot x}\varphi(k,[x]), \tag{2.11}$$

where $[\,\cdot\,]$ refers to the a.e. unique decomposition $x=\gamma_x+[x]$, with $\gamma_x\in\Gamma$ and $[x]\in M$.

As already mentioned, the advantage of this construction is that the transformed hamiltonian is a fibered operator over M^*. Indeed, for the Zak transform of the hamiltonian operator (2.3) one finds

$$\mathcal{U}_{\mathrm{Z}} H \mathcal{U}_{\mathrm{Z}}^{-1} = \int_{M^*}^{\oplus} dk\, H(k) \tag{2.12}$$

with fiber operator

$$H(k) = \frac{1}{2}\big(-\mathrm{i}\nabla_y + k\big)^2 + V_\Gamma(y)\,, \quad k \in M^*\,. \tag{2.13}$$

By Assumption 1, for fixed $k \in M^*$, the operator $H(k)$ acts on $L^2(M)$ with the Sobolev space $H^2(M)$ as domain independently of $k \in M^*$. Each fiber operator $H(k)$ has pure point spectrum accumulating at infinity. For definiteness the eigenvalues are enumerated according to their magnitude $E_0(k) \leq E_1(k) \leq E_2(k) \leq \ldots$ and repeated according to their multiplicity. $E_n : M^* \to \mathbb{R}$ is the n-th energy band function. It is continuous on M^* when viewed as a d-torus. Generically the eigenvalues $E_n(k)$ are non-degenerate. Of course, there may be particular points in k-space where particular energy bands touch each other and the corresponding eigenvalue becomes degenerate. The normalized eigenfunction corresponding to $E_n(k)$ is the Bloch function and denoted by $\varphi_n(k) \in H^2(M)$. It is determined only up to a k-dependent phase factor. A further arbitrariness comes from points where energy bands touch. We denote by $P_n(k)$ the projection along $\varphi_n(k)$ and set

$$P_n = \int_{M^*}^{\oplus} dk P(k)\,, \qquad \mathcal{H}_n = P_n L^2(\mathbb{R}^d)\,. \tag{2.14}$$

Through the Zak transform we have achieved the product structure

$$\mathcal{H} = \mathcal{H}_{\mathrm{s}} \otimes \mathcal{H}_{\mathrm{f}}\,, \qquad \mathcal{H}_{\mathrm{s}} = L^2(M^*)\,,\ \mathcal{H}_{\mathrm{f}} = L^2(M)\,. \tag{2.15}$$

$\psi \in \mathcal{H}_{\mathrm{n}}$ is of the form $\phi(k)\varphi_n(k, y)$. The band index n fixes the local pattern of the wave function ψ while $\phi(k)$ provides the slow variation. Therefore $L^2(M^*)$ is the Hilbert space of the slow degrees of freedom. On the other hand for fixed k, one has oscillations in time determined by the eigenvalues $E_n(k)$. On long time scales, these become fast oscillations. Therefore $\mathcal{H}_{\mathrm{f}} = L^2(M)$ is the Hilbert space of the fast degrees of freedom.

Since $[P_n, H] = 0$, the subspaces $\mathcal{H}_n$ are invariant under $\mathrm{e}^{-\mathrm{i}Ht}$. $P_n \mathrm{e}^{-\mathrm{i}Ht} P_n$ is unitarily equivalent to multiplication by $\mathrm{e}^{-\mathrm{i}E_n(k)t}$ on $L^2(M^*)$. Note that, in general, $\mathcal{H}_n$ is not a spectral subspace for H. The band functions generically have overlapping ranges. Therefore, if slowly varying terms are added to the hamiltonian, the dynamics can no longer be captured so easily by a spectral analysis of the perturbed hamiltonian.

2.2 The magnetic Bloch hamiltonian

We consider $d = 3$. The hamiltonian reads

$$H = \frac{1}{2}\big(-i\nabla_x - A(x)\big)^2 + V_\Gamma(x)\,, \quad x \in \mathbb{R}^3\,, \tag{2.16}$$

with $A(x) = -\frac{1}{2}B \wedge x$, $B \in \mathbb{R}^3$. Physically the most relevant case is $d = 2$. It is included here by setting $x = (x_1, x_2, 0)$ and $B = (0, 0, B_0)$. Following Zak [Zak64], see also [DGR02], one introduces the magnetic translations

$$(T_\alpha\psi)(x) = \big(e^{-i\alpha\cdot(-i\nabla_x + A(x))}\psi\big)(x) = e^{i\alpha A(x)}\psi(x-\alpha) \tag{2.17}$$

with $\alpha \in \mathbb{R}^3$. They satisfy the Weyl relations

$$T_\alpha T_\beta = e^{-\frac{i}{2}B\cdot(\alpha\wedge\beta)}T_{\alpha+\beta} = e^{-iB\cdot(\alpha\wedge\beta)}T_\beta T_\alpha\,. \tag{2.18}$$

To have a commuting subfamily we need

Assumption 2. *The magnetic field B is such that $B\cdot(\gamma\wedge\gamma') \in 2\pi\mathbb{Q}$ for all $\gamma, \gamma' \in \Gamma$.*

In the two-dimensional case our assumption requires that the magnetic flux per unit cell, $B_0\cdot(\gamma_1\wedge\gamma_2)$, is a rational multiple of 2π.

Under the Assumption 2 there exists a sublattice $\Gamma_0 \subset \Gamma$ such that $B\cdot(\gamma\wedge\gamma') \in 2\pi\mathbb{Z}$ for every $\gamma, \gamma' \in \Gamma_0$. Γ_0 is not unique. The set $\{T_\alpha\}_{\alpha\in\Gamma_0}$ is a family of commuting operators, which commute with H. Since $T_\alpha T_\beta = \pm T_{\alpha+\beta}$, the magnetic translations still form only a projective group. It becomes a group by an even smaller sublattice $\Gamma_1 \subset \Gamma_0$ such that $B\cdot(\gamma\wedge\gamma') \in 4\pi\mathbb{Z}$ for all $\gamma, \gamma' \in \Gamma_1$. Another common choice is a further modification of the phase through

$$\mathcal{T}_\alpha = e^{-\frac{i}{2}\varphi(\alpha)}T_\alpha \tag{2.19}$$

with $\varphi(\alpha) = B_1\alpha_2\alpha_3 + B_3\alpha_1\alpha_2 - B_2\alpha_1\alpha_3$. Then $\mathcal{T}_\alpha\mathcal{T}_\beta = \mathcal{T}_{\alpha+\beta}$ for all $\alpha, \beta \in \Gamma_0$.

We can now proceed as in the non-magnetic case. The Zak transform becomes

$$(\mathcal{U}_{\mathrm{Z}}\psi)(k, x) = \sum_{\gamma\in\Gamma_0} e^{-ik\cdot(x+\gamma)}\mathcal{T}_\gamma\psi(x)\,, \quad (k, x) \in \mathbb{R}^6\,. \tag{2.20}$$

The properties of $\mathcal{U}_{\mathrm{Z}}\psi$ are as in (2.2), (2.3) provided Γ is replaced by Γ_0, and $\mathcal{H}_\tau$ is replaced by $\mathcal{H}^B_\tau = \{u \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}}) : (2.23) \text{ below holds true}\}$. In particular, H of (2.16) admits the fiber decomposition

$$\mathcal{U}_{\mathrm{Z}} H \mathcal{U}_{\mathrm{Z}}^{-1} = \int_{M^*}^{\oplus} dk H(k) \tag{2.21}$$

with M^* the first Brillouin zone of Γ_0^* and with the fiber operator

$$H(k) = \frac{1}{2}(-i\nabla_y + \frac{1}{2}B\wedge y + k)^2 + V_\Gamma(y)\,. \tag{2.22}$$

The domain of $H(k)$ is independent of k but, in contrast to $H(k)$ from (2.13), a function u in the domain has to satisfy the more complicated boundary condition

$$e^{-\frac{i}{2}y\cdot(\alpha\wedge B)}u(y-\alpha)=u(y)\,. \tag{2.23}$$

2.3 Dirac hamiltonian, spin-orbit coupling

The Dirac hamiltonian with periodic potential reads

$$H=\beta-i\alpha\cdot\nabla_x+V_\Gamma(x)\,, \tag{2.24}$$

where we have set $m_{\rm e}=1$, $c=1$. As for the Bloch hamiltonian, H admits the fiber decompositon

$$H=\int_{M^*}^{\oplus}dkH(k) \tag{2.25}$$

with fiber hamiltonian

$$H(k)=\beta+\alpha\cdot(-i\nabla_y+k)+V_\Gamma(y)\,. \tag{2.26}$$

$H(k)$ acts on $L^2(M,\mathbb{C}^4)$ with periodic boundary conditions (2.5). The free Dirac operator has a spectral gap of size 2, in our units, between the electron and positron subspace. If we assume $\|V_\Gamma\|<1$, then this gap persists and the eigenvalues can be labelled as $E_0(k)\le E_1(k)\le\dots$ in the electron subspace and as $E_{-1}(k)\ge E_{-2}(k)\ge\dots$ in the positron subspace. One has $E_{-1}(k)<E_0(k)$ for all $k\in M^*$. (In fact the labelling can be achieved without a restriction on $\|V_\Gamma\|$, see [Mau03]).

For $V_\Gamma=0$, the eigenvalue $E(k)$ is two-fold degenerate reflecting the spin $\frac{1}{2}$ of the electron, resp. positron. This degeneracy persists if the periodic potential is inversion symmetric, see [Mau03] for details.

Proposition 2.1. *Let H be given by (2.24) with $\|V_\Gamma\|<1$. Let there exist $a\in\mathbb{R}^3$ such that $V_\Gamma(x+a)=V_\Gamma(-x+a)$. Then each $E_n(k)$ is at least two-fold degenerate.*

Proof. Without loss of generality we may assume $a=0$. We use the standard basis for the α-matrices, see [Tha94]. In this basis time-reversal symmetry is implemented by the anti-unitary operator

$$T\psi(y)=-i\alpha_3\alpha_1\psi^*(y)\,, \tag{2.27}$$

where the complex conjugation is understood component-wise. Using that $\alpha_\ell\alpha_3\alpha_1=-\alpha_3\alpha_1\overline{\alpha}_\ell$, $\ell=1,2,3$, where $\overline{\alpha}_\ell$ refers to matrix element-wise complex conjugation, one checks that

$$-i\nabla_y\alpha_\ell T=-iT\nabla_y\alpha_\ell\,,\quad k\alpha_\ell T=-Tk\alpha_\ell \tag{2.28}$$

and therefore

$$T^{-1}H(k)T = H(-k)\,. \tag{2.29}$$

Secondly we use space inversion as

$$R\psi(y) = \beta\psi(-y)\,. \tag{2.30}$$

Then

$$R^{-1}H(k)R = H(-k)\,. \tag{2.31}$$

Combining both symmetries implies

$$T^{-1}R^{-1}H(k)RT = H(k)\,. \tag{2.32}$$

If $H(k)\psi = E\psi$, then also $RT\psi$ is an eigenfunction with the same eigenvalue. Thus our claim follows from $\langle\psi, RT\psi\rangle = 0$. To verify this identity we note that $-i\alpha_3\alpha_1 = \mathrm{diag}\,(\sigma_2, \sigma_2)$ and $\langle\chi, R\sigma_2\chi^*\rangle = 0$ for an arbitrary two-spinor χ.

Corollary 2.2. *The eigenvalue $E_n(0)$ of $H(0)$ is at least two-fold degenerate.*

Proof. Since $T^*H(0)T = H(0)$ by (2.29) and $\langle\psi, (-i\alpha_3\alpha_1)\psi^*\rangle = 0$, the claim follows.

If V_Γ is not inversion symmetric, generically an energy band is two-fold degenerate at $k = 0$ and then splits into two non-degenerate bands. Note that a non-degenerate eigenvalue $E_n(k)$ has an associated eigenvector with a definite spin orientation.

The Pauli equation with spin-orbit coupling has the hamiltonian

$$H = -\frac{1}{2}\Delta_x + V_\Gamma(x) + \frac{1}{4}\sigma\cdot\big(\nabla V_\Gamma(x)\wedge(-i\nabla_x)\big)\,. \tag{2.33}$$

After Zak transform the corresponding fiber hamiltonian becomes

$$H(k) = \frac{1}{2}(-i\nabla_y + k)^2 + V_\Gamma(y) + \frac{1}{4}\sigma\cdot\big(\nabla V_\Gamma(y)\wedge(-i\nabla_y + k)\big) \tag{2.34}$$

with periodic boundary conditions. H of (2.33) is bounded from below. But otherwise the band structure is similar to the periodic Dirac operator. Proposition 2.1 and Corollary 2.25 hold as stated. In the proof one only has to use the appropriate time-reversal operator, which is $T\psi = \sigma_2\psi^*$ in the σ_3-eigenbasis.

2.4 Gap condition and smoothness

Let us consider one of the periodic hamiltonians, H_{per}, with fiber decomposition $H(k)$. H_{per} is adiabatically perturbed to H^ε. Very crudely the corresponding unitary groups should be close. To make such a notion quantitative a gap condition must be imposed. We denote by $\sigma(H)$ the spectrum of the self-adjoint operator H.

Gap condition: *We distinguish a family of m physically relevant energy bands $\{E_j(k)\,,\ n \le j \le n+m-1\} = \sigma_0(k)$. This family satisfies the gap condition if*

$$\operatorname{dist}\{\sigma_0(k)\,,\ \sigma(H(k)) \setminus \sigma_0(k)\} \ge g > 0 \quad \text{for all } k \in M^*\,. \tag{2.35}$$

We repeat that the gap condition is not a spectral condition for $H_{\rm per}$. Let us set $P^0 = \bigoplus_{j=n}^{n+m-1} P_j$.

Under the gap condition the projector $P(k)$ depends smoothly, in many cases even (real) analytically, on k. $\operatorname{Ran} P^0(k)$ is spanned by the basis $\{\varphi_j(k)\}_{j=n,\dots,n+m-1}$. If the m relevant energy bands have no crossings amongst each other, then φ_j is necessarily an eigenvector of $H(k)$ satisfying $H(k)\varphi_j(k) = E_j(k)\varphi_j(k)$. But if there are band crossings, it can be convenient not to insist on $\varphi_j(k)$ being an eigenvector of $H(k)$. Thus, while $P^0(k)$ is unique, the spanning basis is not. In applications it is of importance to know whether there is at least some choice of $\varphi_j(k)$, $j = n, \dots, n+m-1$, such that they have a smooth k-dependence. Locally, this can be achieved. However, since M^* has the topology of a torus, a global extension might be impossible. In fact this will generically happen for the magnetic Bloch hamiltonian, see [DN80, No81, Lys85] for examples. Somewhat surprisingly, a reasonably general answer has been provided only recently [Pan06]. For the case of the Bloch hamiltonian, analyticity has been proved before in cases $d = 1$, m arbitrary, and d arbitrary, $m = 1$, see Nenciu [Nen83, Nen91] and Helffer, Sjöstrand [HS89]. They rely on analytical techniques. In [Pan06] topological methods are developed.

Proposition 2.3. *In case of the non-magnetic Bloch hamiltonian let either $d \le 3$, $m \in \mathbb{N}$ or $d \ge 4$, $m = 1$. Then there exists a collection of smooth maps $\mathbb{R}^d \ni k \mapsto \varphi_j(k) \in L^2(M)$, $j = n, \dots, n+m-1$, with the following properties*

(i) the family $\{\varphi_j(k)\}_{j=n,\dots,n+m-1}$ is orthonormal and spans the range of $P^0(k)$.

(ii) each map is equivariant in the sense that

$$\varphi_j(k) = \tau(\lambda)\varphi(k+\lambda) \quad \textit{for all } k \in \mathbb{R}^d\,,\ \lambda \in \Lambda\,, \tag{2.36}$$

where $\tau(\lambda)$ is multiplication by $e^{i\lambda\cdot y}$. The same property holds for the non-magnetic periodic Dirac operator and Pauli operator with spin-orbit coupling.

Remark. The proof uses the first Chern class of the vector bundle whose fiber at k is the span of the family $\{\varphi_j(k)\}_{j=n,\dots,n+m-1}$ i.e. $\operatorname{Ran} P^0(k)$. To establish continuity, and thus smoothness, this first Chern class has to vanish, a property, which does not hold for a magnetic Bloch hamiltonian except for some particular energy bands.

If ε is small, excitations across the energy gap are difficult to achieve. More precisely to P^0 one can associate a projection operator Π^ε such that for arbitrary $\ell, \ell' \in \mathbb{N}$, $\tau \in \mathbb{R}_+$, it holds

$$\|(1-\Pi^\varepsilon)e^{-iH^\varepsilon t}\Pi^\varepsilon\psi\| \le c_{\ell,\ell'}(\tau)\varepsilon^\ell\|\psi\| \tag{2.37}$$

for $0 \le t \le \varepsilon^{-\ell'}\tau$ with suitable constants $c_{\ell,\ell'}(\tau)$ independent of ε. In other words that the subspaces $\Pi^\varepsilon\mathcal{H}$ and $(1-\Pi^\varepsilon)\mathcal{H}$ almost decouple, i.e. decouple at any prescribed level of precision and over any polynomial length of the time span under consideration. For the specific case of the Bloch hamiltonian more quantitative details on the decoupling are provided in Section 3.

If the gap condition is not satisfied, the dynamical properties are much more model dependent. Firstly the gap condition can be violated in various ways. In our context, since $H(k)$ has discrete spectrum, the violation comes through band crossings. The behavior close to a band crossing has to be studied separately [LT05, BT05]. In other models the energy band sits at the bottom of the continuous spectrum of $H(k)$ without gap [Teu02]. Then an assertion like Equation (2.37) holds only under a suitable restriction to small ℓ, ℓ', usually $\ell, \ell' = 1$ or perhaps $\ell = 2$, $\ell' = 1$.

The inequality (2.37) makes no assertion about the dynamics inside the almost invariant subspace $\Pi^\varepsilon\mathcal{H}$. While there is a general theory available [PST03a], we prefer to discuss the examples separately in the subsequent sections.

3 Nonmagnetic Bloch hamiltonians: Peierls substitution and geometric phase corrections

We discuss in more detail the effective dynamics for the Schrödinger equation with a periodic potential. For concreteness we fix the spatial dimension to be 3. Under Zak transform the nonmagnetic Bloch hamiltonian becomes

$$\mathcal{U}_Z\Big(\frac{1}{2}\big(-i\nabla_x - A(\varepsilon x)\big)^2 + V_\Gamma(x) + \phi(\varepsilon x)\Big)\mathcal{U}_Z^{-1} = H_Z^\varepsilon \tag{3.1}$$

with

$$H_Z^\varepsilon = \frac{1}{2}\big(-i\nabla_y + k - A(i\varepsilon\nabla_k^\tau)\big)^2 + V_\Gamma(y) + \phi(i\varepsilon\nabla_k^\tau)\,. \tag{3.2}$$

Here ∇_k^τ is differentation with respect to k and satisfying the y-dependent boundary conditions (2.6). H_Z^ε is a self-adjoint operator on $L^2_\tau(\mathbb{R}^3, H^2(M))$, compare with (2.8).

In (3.2) we observe that the external potentials couple the fibers. To emphasize this feature we think of (3.2) as being obtained through Weyl quantization from the operator valued function

$$H_0(k,r) = \frac{1}{2}\big(-i\nabla_y + k - A(r)\big)^2 + V_\Gamma(y) + \phi(r) \tag{3.3}$$

as defined on $(r,k) \in \mathbb{R}^6$ and acting on $\mathcal{H}_\mathrm{f}$ with fixed domain $H^2(M)$, see [PST03b] for details. In this form one is reminded of the Weyl quantization

of the classical hamiltonian function $h_{\rm cl}(q,p) = \frac{1}{2}p^2 + V(q)$ which yields the semiclassical hamiltonian

$$H_{\rm sc} = \frac{1}{2}(-i\varepsilon\nabla_x)^2 + V(x) \tag{3.4}$$

acting in $L^2(\mathbb{R}^3)$. The analysis of (3.4) yields that on the time-scale $\varepsilon^{-1}t$ the wave packet dynamics governed by $H_{\rm sc}$ well approximates the flow generated by $h_{\rm cl}$. In contrast, the adiabatic analysis deals with operator valued symbols, as in (3.3), and has as a goal to establish that the dynamics decouples into almost invariant subspaces and to determine the approximate dynamics within each such subspace.

To be specific, let us then fix throughout one band index n and let us assume that the band energy E_n is nondegenerate and satisfies the gap condition. Therefore we know that $E_n : M^* \to \mathbb{R}$ is smooth and we can choose the family of Bloch functions $\varphi_n(k)$, with $H(k)\varphi_n(k) = E_n(k)\varphi_n(k)$, such that φ_n depends smoothly on k. For each $\ell \in \mathbb{N} = \{0, 1, \ldots\}$ there exists then an orthogonal projection Π_ℓ^ε on $\mathcal{H}_\tau$ such that

$$\|[H_Z^\varepsilon\,,\,\Pi_\ell^\varepsilon]\| \leq c_\ell \varepsilon^{\ell+1} \tag{3.5}$$

for some constants c_ℓ. Integrating in time one concludes that the subspaces $\Pi_\ell^\varepsilon \mathcal{H}_\tau$ are almost invariant in the sense that

$$\|(1-\Pi_\ell^\varepsilon)e^{-i\varepsilon^{-\ell'}tH_Z^\varepsilon}\Pi_\ell^\varepsilon\psi\| \leq \|\psi\|(1+|t|)c_\ell\,\varepsilon^{\ell+1}\varepsilon^{-\ell'} \tag{3.6}$$

for any $\ell, \ell' \in \mathbb{N}$. Note that the adiabatic time scale, order $\varepsilon^{-\ell'}$, can have any power law increase, at the expense of choosing the order of the projection Π_ℓ^ε sufficiently large. Only for times of order $e^{1/\varepsilon}$ one observes transitions away from the almost invariant subspace. The zeroth order projection is attached to the n-th band under consideration, while the higher orders are successively smaller corrections to Π_0^ε. To construct Π_0^ε one considers the projection onto the n-th band, $|\varphi_n(k)\rangle\langle\varphi_n(k)|$, as an operator valued function with values in $B(\mathcal{H}_{\rm f})$. From it we obtain the minimally substituted projection $|\varphi_n(k-A(r))\rangle\langle\varphi_n(k-A(r))|$. Its Weyl quantization is ε-close to the orthogonal projection Π_0^ε.

The second task is to determine the approximate time-evolution on $\Pi_\ell^\varepsilon\mathcal{H}_\tau$. Since the subspace changes with ε, it is more convenient to unitarily map $\Pi_\ell^\varepsilon\mathcal{H}_\tau$ to an ε-independent reference Hilbert space, which in our case is simply $L^2(M^*)$. The dynamics on $L^2(M^*)$ is governed by an effective hamiltonian. It is written down most easily in terms of a hamiltonian function $h_\ell^\varepsilon : M^* \times \mathbb{R}^3 \to \mathbb{R}$. h_ℓ^ε is a smooth function. We also may regard it as defined on $\mathbb{R}^3 \times \mathbb{R}^3$ and Γ^*-periodic in the first argument. h_ℓ^ε admits the power series

$$h_\ell^\varepsilon = \sum_{j=0}^{\ell} \varepsilon^j h_j \tag{3.7}$$

with ε-independent functions h_j. The effective quantum hamiltonian is obtained from h_ℓ^ε through Weyl quantization. The index ℓ regulates the time scale over which the approximation is valid and the size of the allowed error.

In [PST03b] we provide an iterative algorithm to compute h_j. In practice only h_0 and h_1 can be obtained, at best h_2 under simplifying assumptions. While this may look very restrictive, it turns out that already h_1 yields novel physical effects as compared to h_0. Even higher order corrections seem to be less significant.

To lowest order one obtains

$$h_0(k,r) = E_n(k - A(r)) + \phi(r)\,, \tag{3.8}$$

which Weyl-quantizes to

$$\mathcal{W}^\varepsilon[h_0] = E_n(k - A(i\varepsilon\nabla_k)) + \phi(i\varepsilon\nabla_k) \tag{3.9}$$

acting on $L^2(M^*)$, where $i\nabla_k$ is the operator of differentiation with periodic boundary conditions. (The twisted boundary conditions appearing in (3.2) are absorbed into the unitary map of $\Pi_0^\varepsilon\mathcal{H}$ to $L^2(M^*)$.) In solid state physics the Weyl quantization (3.9) is referred to as *Peierls substitution*. (3.8), (3.9) have a familiar form. The periodic potential merely changes the kinetic energy $\frac{1}{2}k^2$ of a free particle to $E_n(k)$. The main distinctive feature is the periodicity of the kinetic energy. For example, in presence of a linear potential ϕ, $\phi(x) = -E\cdot x$, an electron, initially at rest, will start to accelerate along E but then turns back because of periodicity in k.

To first order the effective hamiltonian reads

$$h_1(k,r) = \big(\nabla\phi(r) - \nabla E_n(\widetilde{k}) \wedge B(r)\big)\cdot\mathcal{A}_n(\widetilde{k}) - B(r)\cdot\mathcal{M}_n(\widetilde{k})\,, \tag{3.10}$$

with the kinetic wave number $\widetilde{k} = k - A(r)$. The coefficients $\mathcal{A}_n$ and $\mathcal{M}_n$ are the geometric phases. They carry information on the Bloch functions $\varphi_n(k)$. $\mathcal{A}_n$ is the Berry connection given through

$$\mathcal{A}_n(k) = i\langle\varphi_n(k)\,,\ \nabla_k\varphi_n(k)\rangle_{\mathcal{H}_f} \tag{3.11}$$

and $\mathcal{M}_n$ is the Rammal-Wilkinson phase given trough

$$\mathcal{M}_n(k) = \frac{1}{2}i\langle\nabla_k\varphi_n(k), \wedge(H(k) - E_n(k))\nabla_k\varphi_n(k)\rangle_{\mathcal{H}_f}\,. \tag{3.12}$$

The Bloch functions φ_n are only determined up to a smooth phase $\alpha(k)$, i.e. instead of $\varphi_n(k)$ one might as well use $e^{-i\alpha(k)}\varphi_n(k)$ with smooth $\alpha : M^* \to \mathbb{R}$. Clearly $\mathcal{M}_n$ is independent of the gauge field α. On the other hand, $\mathcal{A}$ is gauge-dependent while its curl

$$\Omega_n = \nabla \wedge \mathcal{A}_n \tag{3.13}$$

is gauge independent. From time-reversal one concludes that

$$\Omega_n(-k) = -\Omega_n(k)\,. \tag{3.14}$$

In particular, in dimension $d = 2$ for the first Chern number of the Bloch vector bundle one obtains

$$\int_{M^*} dk\Omega_n(k) = 0\,. \tag{3.15}$$

For the magnetic Bloch hamiltonian, (3.14) is violated in general, see Section 4. The integral in (3.15) can take only integer values (in the appropriate units) and the first Chern number may be different from zero. Physically this leads to the quantization of the Hall current [PST03b, SN99].

We still owe the reader precise a statement on the error in the approximation. At the moment we work in the representation space at precision level $\ell = 1$. Let $H_{\rm eff}$ be the Weyl quantization of $h_0 + \varepsilon h_1$, see (3.8) and (3.10). There is then a unitary $U^\varepsilon : \Pi_1^\varepsilon \mathcal{H}_\tau \to L^2(M^*)$ such that for all $\psi \in \mathcal{H}_\tau$

$$\|\big(e^{-iH_Z^\varepsilon t} - U^{\varepsilon *} e^{-iH_{\rm eff} t} U^\varepsilon\big)\Pi_1^\varepsilon \psi\| \leq c\|\psi\|(1+|\tau|)\varepsilon^2 \tag{3.16}$$

with $|t| \leq \varepsilon^{-1}\tau$ and some constant c independent of $\|\psi\|$, τ, and ε.

4 Magnetic Bloch hamiltonians: the Hofstadter butterfly

We turn to a magnetic Bloch hamiltonian in the form (1.4), in dimension $d = 2$ and with a transverse constant magnetic field B_0. We want to explain how the limits $B_0 \to \infty$ and $B_0 \to 0$ can be understood with adiabatic methods. As a remark, it is worthwhile to recall that, when the physical constants are restored, the dimensionless parameter B_0 is given by

$$B_0 = \frac{\mathcal{B}_0 S}{2\pi\hbar c/e}\,, \tag{4.1}$$

where S is the area of the fundamental cell of Γ and $\mathcal{B}_0$ the strength of the magnetic field, both expressed in their dimensional units. Thus B_0 corresponds physically to the magnetic flux per unit cell divided by hc/e, as the fundamental quantum of magnetic flux. This section is based essentially on [FP06], which elaborates on previous related results [Bel86, HS89].

Adiabatic limits are always related to separation of time-scales. In the present case, one indeed expects that as $B_0 \to \infty$ the cyclotron motion induced by B_0 is faster than the motion induced by V_Γ, while in the limit $B_0 \to 0$ the microscopic variations of the wave function induced by V_Γ are expected to be faster than the cyclotron motion.

Let us focus first on the Landau regime $B_0 \to \infty$. In order to make quantitative the previous claim, one introduces the operators

$$\begin{cases} L_1 = \frac{1}{\sqrt{B_0}}\left(p_1 + \frac{1}{2}B_0\, x_2\right)\,, \\ \\ L_2 = \frac{1}{\sqrt{B_0}}\left(p_2 - \frac{1}{2}B_0\, x_1\right)\,, \end{cases} \qquad [L_1, L_2] = i\mathbf{1}, \tag{4.2}$$

and the complementary pair of operators

$$\begin{cases} G_1 = \frac{1}{B_0}\left(p_1 - \frac{1}{2}B_0\, x_2\right), \\ \\ G_2 = \frac{1}{B_0}\left(p_2 + \frac{1}{2}B_0\, x_1\right), \end{cases} \qquad [G_1, G_2] = \tfrac{i}{B_0}\mathbf{1}, \tag{4.3}$$

where the relative sign is chosen such that $[L_i, G_j] = 0$, for $i, j = 1, 2$.

If $V_\Gamma = 0$, then $H_{\rm MB}$ describes a harmonic oscillator, with eigenfunctions localized on a scale $|B_0|^{-1/2}$; this corresponds to the cyclotron motion in classical mechanics. Since $[G_i, H_{\rm MB}] = 0$, the operators G_1 and G_2 describe conserved quantities, which semiclassically correspond to the coordinates of the center of the cyclotron motion.

If $V_\Gamma \neq 0$, but the energy scale $\|V_\Gamma\|$ is smaller than the cyclotron energy $\approx B_0$, then the operators G_i have a non-trivial but slow dynamics. By introducing the adiabatic parameter $\eta = 1/B_0$ the hamiltonian reads

$$H_{\rm MB} = \frac{1}{2\eta}\left(L_1^2 + L_2^2\right) + V_\Gamma\left(G_2 - \sqrt{\eta}L_2,\, -G_1 + \sqrt{\eta}L_1\right). \tag{4.4}$$

In view of the commutator $[G_1, G_2] = i\eta\mathbf{1}$, one can regard $\eta\, H_{\rm MB}$ as the η-Weyl quantization (in the sense of the mapping $(q,p) \mapsto (G_1, G_2)$) of the operator-valued symbol

$$h_{\rm MB}(q,p) = \frac{1}{2}\left(L_1^2 + L_2^2\right) + \eta\, V_\Gamma\left(p - \sqrt{\eta}L_2, -q + \sqrt{\eta}L_1\right). \tag{4.5}$$

For each fixed $(q,p) \in \mathbb{R}^2$, $h_{\rm MB}(q,p)$ is an operator acting in the Hilbert space $\mathcal{H}_{\rm f} \cong L^2(\mathbb{R})$ corresponding to the fast degrees of freedom. If $\|V_\Gamma\|_{\mathcal{B}(\mathcal{H})} < \infty$, then $h_{\rm MB}(q,p)$ has purely discrete spectrum, with eigenvalues

$$\lambda_{n,\,\eta}(q,p) = (n + \frac{1}{2}) + \eta V_\Gamma(p, -q) + \mathcal{O}(\eta^{3/2}), \qquad n \in \mathbb{N},$$

as $\eta \downarrow 0$. The index $n \in \mathbb{N}$ labels the *Landau levels*. For η small enough, each eigenvalue band is separated from the rest of the spectrum by an uniform gap. Thus we can apply space-adiabatic perturbation theory to show that the band corresponds to an almost-invariant subspace $\Pi_{n,\eta} L^2(\mathbb{R}^2)$. Let us focus on a specific $n \in \mathbb{N}$. One can prove that the dynamics inside $\mathrm{Ran}\, \Pi_{n,\eta} L^2(\mathbb{R}^2)$ is described by an effective hamiltonian, which at the first order of approximation in η reads

$$h_1^\eta = (n + \frac{1}{2}) + \eta V_\Gamma(G_1, -G_2). \tag{4.6}$$

The first term in (4.6) is a multiple of the identity, and as such does not contribute to the dynamics as far as the expectation values of observables are concerned. Leading-order dynamics is thus described by the second term, which does not depend on the Landau level $n \in \mathbb{N}$. Since V_Γ is a biperiodic function and (G_1, G_2) a canonical pair, the second term is a Harper-like

operator. The spectrum of such operators exhibit a complex fractal behavior (*Hofstadter butterfly*) sensitively depending on the diophantine properties of $\alpha = \frac{B_0}{2\pi}$ (notice that $V_\Gamma(G_1, G_2)$ depends on α through the commutator $[G_1, G_2] = iB_0^{-1}\mathbf{1}$). The Cantor structure of the spectrum was proven first in [BS82] for the case $V_\Gamma(x_1, x_2) = \lambda \cos x_1 + \cos x_2$ (Harper model), for a dense set of the parameter values. Later Helffer and Sjöstrand accomplished a detailed semiclassical analysis of the Harper operator [HS89]. As a final step the Cantor spectrum has been proven by Puig ($\lambda \neq 0$, α Diophantine) [Pu04], and by Avila and Jitomirskaya [AJ05] for all the conjectured values of the parameters: $\lambda \neq 0$, α irrational (the *Ten Martini conjecture*, as baptized by B. Simon).

Secondly we turn to the opposite limit $B_0 \to 0$, where the slow part of the dynamics is still described by the magnetic momentum operators $\widetilde{L}_j = \sqrt{B_0} L_j$ ($j = 1, 2$), with commutator of order $\mathcal{O}(B_0)$. However the decomposition given by (4.2) and (4.3) is no longer convenient.

Since A_0 is a linear function, $A_0(\varepsilon x) = \frac{1}{2}\varepsilon B_0 \wedge x$, the slow variation limit $\varepsilon \to 0$ agrees with the weak field limit $B_0 \to 0$. We then pose $\varepsilon = B_0$ and we regard H_{MB} in (1.4) as an adiabatic perturbation of the periodic hamiltonian (2.3). Thus we are reduced to the situation described in Section 3: to each isolated Bloch band of the unperturbed hamiltonian there corresponds a subspace $\Pi_{n,\varepsilon} L^2(\mathbb{R}^2)$ which is approximately invariant under the dynamics as $\varepsilon \downarrow 0$. The dynamics inside this subspace is described by Peierls substitution (3.9), which now reads

$$\mathcal{W}^\varepsilon[h_0] = E_n(k - \frac{1}{2} e_3 \wedge (i\varepsilon\nabla_k)), \tag{4.7}$$

as an operator acting in $L^2(\mathbb{T}^2, dk)$. Here $B_0 = (0, 0, \varepsilon)$ and e_i is the unit vector in the i-th direction.

Formula (4.7) shows that the leading order effective hamiltonian depends only on the operators $(K_1, K_2) = K$,

$$K = k - \frac{1}{2} e_3 \wedge (i\varepsilon\nabla_k),$$

which roughly speaking are the Fourier transform of the pair $(\widetilde{L}_1, \widetilde{L}_2)$, and not on the complementary pair of operators. The same property holds true for the effective hamiltonian h_ℓ^ε, at any order of approximation $\ell \in \mathbb{N}$, see [FP06], with important consequences on the splitting of magnetic subbands at small but finite B_0.

An operator in the form (4.7), shortly written $E_n(K_1, K_2)$, is *isospectral* to an Harper-like operator, namely $E_n(G_1, G_2)$ acting in $L^2(\mathbb{R})$. Indeed the first numerical evidence of the butterfly-like Cantor structure of the spectrum of Harper-like operators appeared when Hofstadter investigated the spectrum of $\cos K_1 + \cos K_2$ as a function of ε [Ho76]. On the other side, an operator of the form $E_n(K_1, K_2)$ is not *unitarily equivalent* to the Harper operator

$E_n(G_1, G_2)$. The important geometric and physical consequences of this fact are developed in [FP06].

Having explained the two extreme cases, $B_0 \to 0$ and $B_0 \to \infty$, the reader may wonder about the intermediate values of the magnetic field, $B_0 \approx 1$. As explained already in Section 2.3 it is convenient to introduce the magnetic translations

$$\mathcal{T}_\alpha = e^{-\frac{i}{2}\varphi(\alpha)} \exp(iB_0\, \alpha \cdot G), \qquad \alpha \in \Gamma_0,$$

see (2.17) and (2.19). If B_0 satisfy Assumption 2, then $\{\mathcal{T}_\alpha\}$ is a commutative group, thus leading to the magnetic Zak transform (2.20). H_{MB} is then a fibered operator over the magnetic Bloch momentum $\kappa \in \mathbb{T}^2$. At each κ the spectrum of $H_{\mathrm{MB}}(\kappa)$ is pure point and the corresponding eigenvalues $\mathcal{E}_n^{B_0}$ are the *magnetic Bloch bands*.

In view of this structure, one might argue that the adiabatic perturbation of the hamiltonian which includes, on top of the constant magnetic field B_0, a slowly varying magnetic potential $A(\varepsilon x)$ as in (1.5) can be treated with the methods of Section 3. There is however one crucial element missing. Indeed one can still associate to each magnetic Bloch band $\mathcal{E}_n^{B_0}$, isolated from the rest of the spectrum, an almost-invariant subspace $\mathrm{Ran}\, \Pi_n^{B_0}$. On the other side the construction of the effective hamiltonian relies on smoothness which may be impeded for topological reasons. Indeed the analogue of Proposition 2.3 is generically false for magnetic Bloch hamiltonians, as well-understood [DN80, No81, Lys85]. In geometric terminology this fact is rephrased by saying that the magnetic Bloch bundle is generically non-trivial (in technical sense). This important fact has sometimes been overlooked. For example, Assumption B in [DGR04] is equivalent to the triviality of the magnetic Bloch bundle. Under this assumption the magnetic case is already covered by the results in [PST03b]. Thus the problem of adiabatic perturbation of a generic magnetic Bloch hamiltonian appears to be an open, in our view challenging, problem for the future.

5 Piezoelectricity

In the year 1880 the brothers Jacques and Pierre Curie discovered that some crystalline solids (like quartz, tourmaline, topaz, ...) exhibit a macroscopic polarization if the sample is strained.

It turns out that also this effect can be understood in the framework of adiabatically perturbed periodic hamiltonians, cf. [PSpT06, Lei05]. The perturbation is now slowly in time,

$$H_{\mathrm{PE}}(t) = -\frac{1}{2}\Delta_x + V_{\Gamma(\varepsilon t)}(x, \varepsilon t)\,. \tag{5.1}$$

If the potential $V_\Gamma(x, \varepsilon t)$ has no center of inversion, i.e. there is no point with respect to which the potential has space-reflection symmetry, then the slow

variation of the periodic potential is expected to generate a non-zero current and can be shown to do so for particular examples [ABL1997]. By translation invariance this current if averaged over a unit cell is everywhere the same and we denote the average current by $J^\varepsilon(t)$. For the following discussion we assume that V_Γ varies only for times in the finite interval $[0,T]$. Integrating the current per volume over the relevant time interval yields the average polarization,

$$\Delta\mathbf{P}^\varepsilon = \int_0^T \mathrm{d}t\, J^\varepsilon(t)\,.$$

In this section we discuss results that relate the current $J^\varepsilon(t)$ directly to the quantum mechanics of non-interacting particles governed by the hamiltonian (5.1), without the detour via the semiclassical model. For this we need to solve the Schrödinger equation with initial state $\rho(0) = P(0)$ being the spectral projection of $H_{\mathrm{PE}}(0)$ below the Fermi energy $E(0)$. Since the piezo effect occurs only for insulators, we can assume that $E(0)$ lies in a gap of the spectrum of $H_{\mathrm{PE}}(0)$ and, in order to simplify the discussion, we also assume that this gap does not close in the course of time. Hence there is a continuous function $E : [0,T] \to \mathbb{R}$ such that $E(t)$ lies in a gap of $H_{\mathrm{PE}}(t)$ for all t. The state at time t is given by

$$\rho^\varepsilon(t) = U^\varepsilon(t,0)\, P(0)\, U^\varepsilon(t,0)^*\,,$$

where the unitary propagator $U^\varepsilon(t,0)$ is the solution of the time-dependent Schrödinger equation

$$\mathrm{i}\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\, U^\varepsilon(t,0) = H_{\mathrm{PE}}(t)\, U^\varepsilon(t,0) \qquad \text{with} \quad U^\varepsilon(0,0) = \mathbf{1}\,. \tag{5.2}$$

With the current operator given by

$$j^\varepsilon := \frac{\mathrm{i}}{\varepsilon}\,[H(t), x] = -\frac{\mathrm{i}}{\varepsilon}\nabla_x\,, \tag{5.3}$$

and the trace per volume defined as

$$\mathcal{T}(A) := \lim_{\Lambda_n \to \mathbb{R}^3} \frac{1}{|\Lambda_n|}\mathrm{Re}\,\mathrm{Tr}(\mathbf{1}_{\Lambda_n} A)\,, \tag{5.4}$$

with $\mathbf{1}_{\Lambda_n}$ being the characteristic function of a 3-dimensional box Λ_n with finite volume $|\Lambda_n|$, the average current in the state $\rho^\varepsilon(t)$ is

$$J^\varepsilon(t) = \mathcal{T}(\rho^\varepsilon(t)\, j^\varepsilon)\,.$$

Finally the average polarization is

$$\Delta\mathbf{P}^\varepsilon = \int_0^T \mathrm{d}t\ \mathcal{T}(\rho^\varepsilon(t)\, J^\varepsilon)\,, \tag{5.5}$$

which is the main quantity of physical interest. The given framework allows us to describe the macroscopic polarization of a solid by a pure *bulk property*, i.e. independently of the shape of the sample.

In the simplest but most important case (see Paragraph (ii) in Section 1 for a discussion of the model), the periodic potential $V_\Gamma(x, \varepsilon t)$ is periodic with respect to a time-*independent* lattice Γ. For this case King-Smith and Vanderbilt [KSV93] derived a formula for $\Delta\mathbf{P}$ based on linear response theory, which turned out to make accurate predictions for the polarization of many materials. Their by now widely applied formula reads

$$\Delta\mathbf{P} = \frac{1}{(2\pi)^3} \sum_{n=0}^{N_c} \int_{M^*} \mathrm{d}k \, \big(\mathcal{A}_n(k,T) - \mathcal{A}_n(k,0)\big), \tag{5.6}$$

where the sum runs over all the occupied Bloch bands and $\mathcal{A}_n(k,t)$ is the Berry connection coefficient for the n-th Bloch band at time $t \in \mathbb{R}$,

$$\mathcal{A}_n(k,t) = \mathrm{i}\langle \varphi_n(k,t), \nabla_k \varphi_n(k,t)\rangle_{L^2(M)} \,.$$

Although $\mathcal{A}_n$ depends on the choice of the Bloch function φ_n, the average polarization (5.6) defines a gauge invariant quantity, i.e. it is independent of the choice of Bloch functions.

In [PSpT06] we show that $\Delta\mathbf{P}^\varepsilon$ defined in (5.5) approaches $\Delta\mathbf{P}$ as given by the King-Smith and Vanderbilt formula (5.6) with errors smaller than any power of ε, whenever the latter is well defined. More precisely we show that under suitable technical conditions on $V_\Gamma(t)$ the average polarization is well defined and that for any $N \in \mathbb{N}$

$$\Delta\mathbf{P}^\varepsilon = -\frac{1}{(2\pi)^d} \int_0^T \mathrm{d}t \int_{M^*} \mathrm{d}k \; \Theta(k,t) + \mathcal{O}(\varepsilon^N) \,, \tag{5.7}$$

where

$$\Theta(k,t) := -\mathrm{i}\,\mathrm{tr}\,\big(P(k,t)\,[\partial_t P(k,t),\, \nabla_k P(k,t)]\,\big) \,, \tag{5.8}$$

and $P(k,t)$ is the Bloch-Floquet fiber decomposition of the spectral projector $P(t) = \mathbf{1}_{(-\infty, E(t)]}(H_{\mathrm{PE}}(t))$. Whenever all Bloch bands within $\mathrm{Ran}P(k,t)$ are isolated, the explicit term in (5.7) agrees with (5.6). Note however that (5.7) is more general, since it can be applied also to situations where band crossings occur within the set of occupied bands.

From the point of view of adiabatic approximation, this result is actually quite simple, since one just needs the standard time-adiabatic theory. At time $t = 0$ the state $\rho(0)$ is just the projection $P(0)$ onto the subspace of the isolated group of occupied bands. Since these bands remain isolated during time evolution, this subspace is adiabatically preserved according to the original adiabatic theorem of Kato [Ka50], i.e.

$$\rho^\varepsilon(t) = P(t) + \mathcal{O}(\varepsilon) \,,$$

and one can compute the higher order corrections to $\rho^\varepsilon(t)$ using the higher order time-adiabatic approximation due to Nenciu [Ne93]. In order to get explicit results, one has to do the adiabatic approximation for each fixed

$k \in M^*$ separately. This is possible since $H_{\mathrm{PE}}(t,k)$ is still fibered in k, due to translation invariance with respect to a time-independent lattice. However, since we need to differentiate with respect to k in order to compute the current, as suggested by formula (5.8), the expansion needs to be done uniformly on spaces of suitable equivariant functions. This makes the proof more technical than expected at first sight.

Alternatively one can derive also for $H_{\mathrm{PE}}(t)$ the semiclassical equations of motion including first order corrections:

$$\begin{cases} \dot{q} = \nabla_k E_n(k,t) - \varepsilon\, \Theta_n(k,t), \\ \dot{k} = 0\,. \end{cases} \tag{5.9}$$

And again averaging the velocity over the first Brillouin zone yields the correct quantum mechanical average current that is the contribution from the n-th band.

Note the striking similarity between the semiclassical corrections in (5.8) and the electromagnetic field. If we define the geometric vector potential

$$\mathcal{A}_n(k,t) = \mathrm{i}\langle \varphi_n(k,t), \nabla_k \varphi_n(k,t)\rangle_{L^2(M)},$$

and the geometric scalar potential

$$\phi_n(k,t) = -\mathrm{i}\langle \varphi_n(k,t), \partial_t \varphi_n(k,t)\rangle_{L^2(M)},$$

in terms of the Bloch function $\varphi_n(k,t)$ of some isolated band, then in complete analogy to the electromagnetic fields we have

$$\Theta_n(k,t) = -\partial_t \mathcal{A}_n(k,t) - \nabla_k \phi_n(k,t), \tag{5.10}$$

and

$$\Omega_n(k,t) = \nabla_k \wedge \mathcal{A}_n(k,t)\,. \tag{5.11}$$

Time-dependent deformations of a crystal generically also lead to a time-dependent periodicity lattice $\Gamma(t)$, see (5.1). This more general situation is considered in [Lei05, LP06]. Now the lattice momentum k is no longer a conserved quantity and the full space-adiabatic perturbation theory is required in order to compute the corresponding piezoelectric current. As a result an additional term appears in the semiclassical equations of motion, reflecting the deformation of the lattice of periodicity.

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